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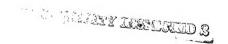
# Demonstration of a Three-Dimensional Numerical Groundwater Flow and Transport Simulation in Savannah River Site, South Carolina

by Bernard B. Hsieh, Mansour Zakikhani, William D. Martin

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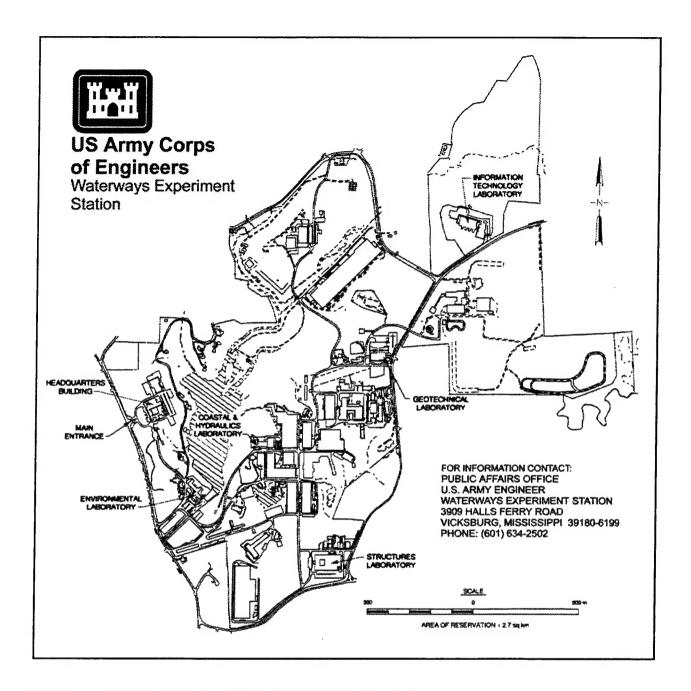
# Demonstration of a Three-Dimensional Numerical Groundwater Flow and Transport Simulation in Savannah River Site, South Carolina

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U.S. Army Corps of Engineers Waterways Experiment Station 3909 Halls Ferry Road Vicksburg, MS 39180-6199

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# **Contents**

Preface	v
1—Introduction	1
Background	1 2
2—Hydrogeologic Description of the Model Area	3
Site Characteristics	3
Hydraulic Properties of Hydrostratigraphic Units	6
Hydrostratigraphic Framework	11
3—Numerical Model Development	13
FEMWATER	13
GMS Interface	13
Mesh generation	14
Boundary conditions	14
Initial conditions	17
Transient flow simulation	17
Transport simulation	26
4—Conclusions	30
References	31
SF 298	
List of Figures	
Figure 1. Regional location and model boundary of SRS	4
Figure 2. Ground surface elevation for the model domain	5
·	5
Figure 3. Regional hydrogeologic system at SRS	6

Figure 4.	Groundwater pumping locations used in the regional model	7
Figure 5.	Hydrologic cycle and water budget at SRS	9
Figure 6.	Potentiometric surface and horizontal groundwater flow directions of the Congaree-Fourmile and Cretaceous Zones at SRS during the first quarter of 1992	12
Figure 7.	Front view of elevation at SRS regional model for N-S direction	15
Figure 8.	2D mesh and borehole locations for SRS regional model	16
Figure 9.	3D computational mesh for SRS regional model	16
Figure 10.	Simulated groundwater flow for top aquifer layer at end of 1-year pumpage dominated simulation	18
Figure 11.	Difference of pressure head distribution between ending time and starting for 1-year pumpage dominated simulation	19
Figure 12.	Simulated groundwater flow for top aquifer layer at end of 1-year infiltration dominated simulation	20
Figure 13.	Difference of pressure head distribution between ending time and starting for 1-year infiltration dominated simulation	21
Figure 14.	Simulated groundwater flow for top aquifer layer at end of two year combined factors	23
Figure 15.	Difference of pressure head distribution between ending time and starting for 2-year combined factors	24
Figure 16.	Difference of pressure head distribution for layer 1 at end of 1-year simulation	25
Figure 17.	Sources of tritium concentrations for SRS regional model (top view)	27
Figure 18.	Cross-sectional view of tritium concentration sources for SRS regional model	27
Figure 19.	Difference of tritium concentration distribution between ending time and starting time for two year transport simulation	29

### **Preface**

Demonstration of a three-dimensional numerical groundwater flow and transport simulation at the Savannah River Site, South Carolina, as documented in this report, was performed for the U.S. Environmental Protection Agency (EPA), National Exposure Research Laboratory, Athens, GA. Mr. Bob Carsel, Regulatory Support Branch, Ecosystems Research Division, National Exposure Research Laboratory, EPA, Athens, GA, was point of contact.

The study was conducted in the Hydraulics Laboratory (HL) and the Environmental Laboratory (EL) of the U.S. Army Engineer Waterways Experiment Station (WES) during the period September 1994 to September 1995 under the direction of Mr. R. A. Sager, Acting Director, HL; Dr. William D. Martin, Acting Chief, Hydro-Science Division, HL; Dr. John Harrison, Director, EL; Dr. John W. Keeley, Assistant Director, EL; Dr. Richard E. Price, Chief, Environmental Processes and Effects Division, EL; and Dr. M. S. Dortch, Chief, Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division, EL.

The study was conducted by Dr. Bernard B. Hsieh, Hydro-Science Division, HL, and Dr. Mansour Zakikhani, WQCMB, EL, and the report was prepared by Drs. Hsieh, Zakikhani, and Martin.

This report is being published by the WES Coastal and Hydraulics Laboratory (CHL). The CHL was formed in October 1996 with the merger of the WES Coastal Engineering Research Center and Hydraulics Laboratory. Dr. James R. Houston is the Director of the CHL, and Messrs. Richard A. Sager and Charles C. Calhoun, Jr., are Assistant Directors.

Dr. Robert W. Whalin was Director of WES during the publication of this report.

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# 1 Introduction

### **Background**

The U.S. Army Engineer Waterways Experiment Station (WES) and Brigham Young University (BYU), Provo, UT, have jointly developed a user-friendly graphical interface for groundwater models, the Groundwater Modeling System (GMS). The U.S. Environmental Protection Agency (EPA) initially contributed to the cost of the GMS development. The GMS (1994) is a pre- and post-processing software for several different groundwater models, including a three-dimensional (3-D) finiteelement model of density-dependent flow and transport through saturatedunsaturated porous media (FEMWATER). The model was developed by G. T. Yeh, Pennsylvania State University (PSU), University Park, PA, and later modified by the WES staff. FEMWATER can handle all the options of the two previous models (LEWASTE and FEMWATER) plus the option of density-driven flow and transport. The input and output structures of the model have been modified by WES to adapt the graphical interface file format. The subject of the study is a cooperative research effort between the EPA Environmental Research Laboratory at Athens, GA (AERL), WES, and PSU. The Savannah River Site (SRS), which contains a point source of groundwater pollution, was selected as the demonstration site for the usability of this tool.

The SRS is located near Aiken, SC. The site has been operated by the U.S. Department of Energy for production of defense-related nuclear materials. Hazardous and radioactive products generated by the plant operations have been stored, buried, or discharged into seepage basins on the plant site (Andersen et al. 1988). The site has been contaminated by point sources of radionuclide isotopes. Several modeling studies of SRS and other nearby areas have been reported in the literature. These studies usually addressed localized problems. Although they provided useful insight to management of water resources in particular areas, they have not tackled site-wide issues. More importantly, no transient and long-term simulations have been reported for the site. The development of a 3-D numerical model has been considered as a useful tool for integrating existing data and testing conditions regarding the nature of the site hydrogeologic system.

The study presented in this report was part of a cooperative research effort between WES, AERL, and PSU. The primary objective of the research was to demonstrate the capability of the GMS to model point source pollution using data from a site at the SRS.

### Scope of Work

The work involved gathering available chemical and hydrogeological data measured at the site. The hydrogeologic data then were used to develop a 3-D conceptual model. The conceptual model was used to set up a numerical mesh system and other input parameters for addressing point sources of contamination at the site. The FEMWATER/GMS finite element flow and transport code was used in all the simulations. Tritium was selected as the chemical of concern at the site because it is part of the water molecules and does not undergo chemical reaction. Effects of hydrogeologic parameters such as infiltration and pumping on flow and tritium transport were investigated. The variation of hydraulic heads and velocities for the modeled area was simulated for 1 year. The results of the flow and transport behavior can be used to perform more detailed analyses of specified management issues in the future. Further research might focus on refinements of the model mesh to allow detailed modeling of flow and transport parameters for water quality at the site.

In this report, the site hydrogeological conditions are briefly described. The application of FEMWATER/GMS to regional and transient modeling of the flow and transport of tritium at the site is discussed. The modeled area covers approximately 1,702 sq km. The modeled domain includes the Hollow Creek and the Upper and Lower Three Runs basins. It is bounded by the Savannah River on the southwest and the Salkehatchie River on the east, and extends north to Aiken, SC. The modeled domain was selected considering the characteristics of the ground surface and historical groundwater flow lines.

# 2 Hydrogeologic Description of the Model Area

### Site Characteristics

The Savannah River Site (SRS) is located in the coastal plain province on the Aiken Plateau (Figure 1). The elevation of this plateau varies from 30 to 120 m above mean sea level. SRS is underlain by a 220- to 380-m-thick, seaward-thickening wedge of coastal plain. The surface elevation of the modeled area is illustrated by the color contour in Figure 2. The figure identifies that Hollow Creek and Three Runs basins are in the relatively low elevations within the modeled area. The wedge of sediments increases in thickness from the fall line toward the coast. The sediments overlying the bedrock consist primarily of sands, silts, and clays with an increase in calcareous marls downdip. Figure 3 shows a cross section of a generalized regional hydrogeology interpretation of the site (Aucott, Davis, and Speiran 1987).

The sediments in the SRS are composed of unconsolidated sands, clayey sands, sandy clays, and lesser amounts of calcareous sediment. The unconsolidated sediments form a multilayered system of aquifers and aquitards. The aquitard units usually consist of clay and silt strata that frequently have limited areal extent (Duffield, Buss, and Stephenson 1990). Although the vertical sequence of hydrostratigraphic units varies across the study area, the hydrogeologic structure from the lowest subsurface layer is generally divided into the Middendorf Aquifer, Black Creek Aquifer, Congaree Formation, Tertiary Sand Aquifer with confined layers in the Peedee Formation, Black Creek Formation, and Congaree Formation on a regional scale. These layers were used to create the model mesh.

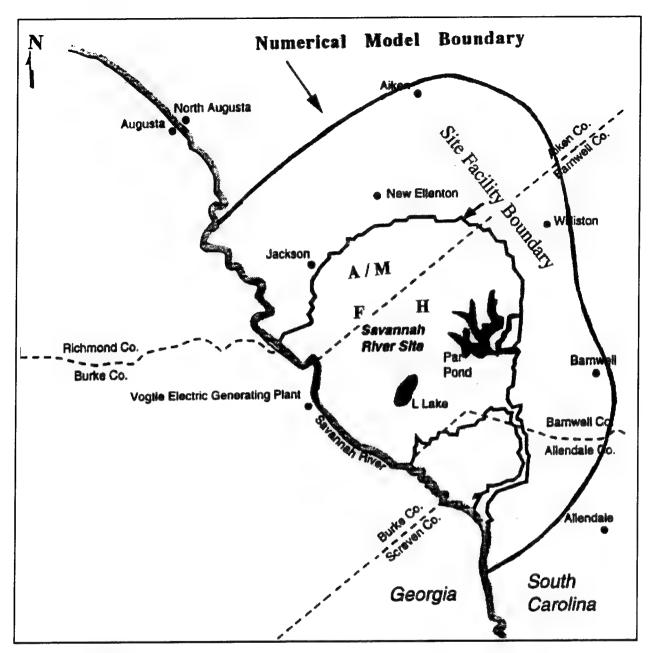


Figure 1. Regional location and model boundary of SRS

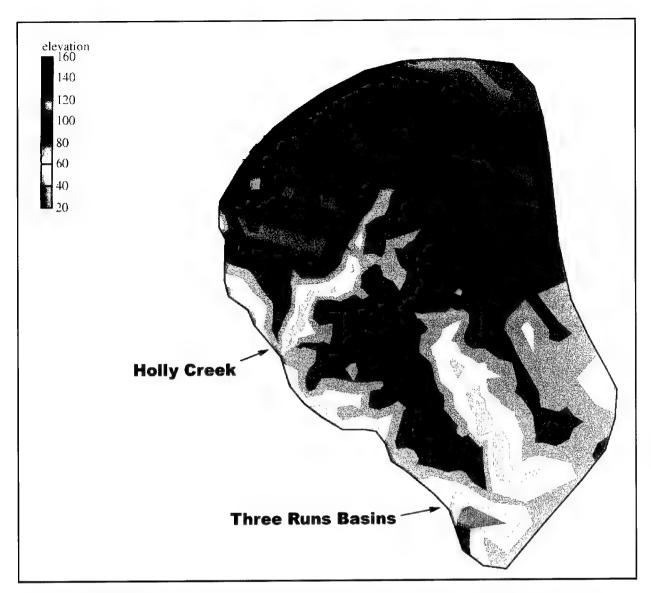


Figure 2. Ground surface elevation for the model domain (elevations are given in meters referred to mean sea level)

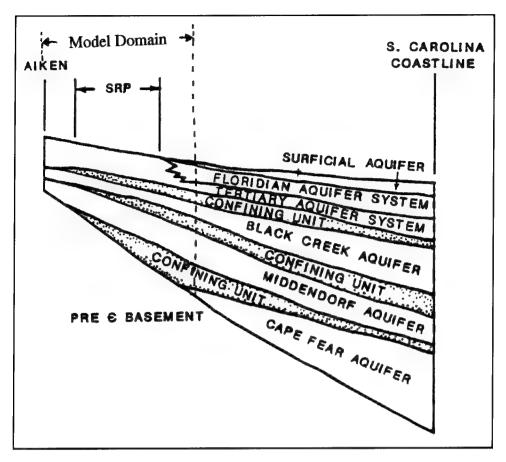


Figure 3. Regional hydrogeologic system at SRS (from Aucott, Davis, and Speiran 1987)

### **Hydraulic Properties of Hydrostratigraphic Units**

Hydraulic property measurements and estimates are available for most of the hydrostratigraphic units underlying SRS. While regional estimates of aquifer parameters are also available from other modeling studies performed in the vicinity of SRS, there is a wide range in hydraulic conductivities within each of the hydrogeographic units. Properties of individual aquifers and aquitards as described in a report by Andersen et al. (1988) are summarized as follows:

- a. Crystalline Metamorphic and Triassic Sedimentary Rock: A representative value of hydraulic conductivity for the crystalline bedrock range is approximately 1.2 x 10<sup>-5</sup> m/d and the values for the Triassic rocks are smaller by 4 orders of magnitude. These are considered to be impermeable materials.
- b. Middendorf Formation: Based on three pump tests in this aquifer, two pump tests in F Area and one in L area (Figure 4), an average transmissivity of 1.5 x 10<sup>3</sup> m<sup>2</sup>/d was obtained. Hydraulic conductivity estimates range from 12.5 m/d to 88.4 m/d in F Area to 28.3 m/d

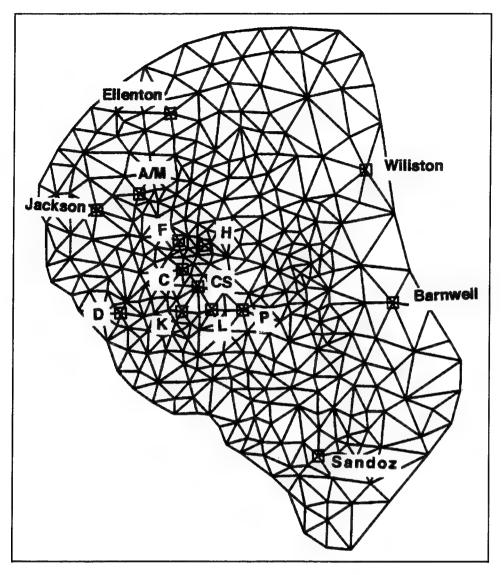


Figure 4. Groundwater pumping locations used in the regional model

28.3 m/d in L Area. According to Logan and Euler (1988), a storage coefficient of  $2.5 \times 10^{-4}$  was obtained from a pump test performed at the Barnwell Nuclear Fuel Plant. The effective porosity estimates for the aquifer are given by Siple (1967) as 0.20 to 0.30.

- c. Black Creek Formation: Little or no data are available on hydraulic property estimates for this formation. Simulated leakage coefficients from Aucott (1988) range from 10<sup>-4</sup>/day to 10<sup>-8</sup>/day. Horizontal hydraulic conductivity estimates used in the General Separations Area (A/M, Figure 4) are 1.8 m/d and 1.5 m/d; vertical hydraulic conductivities estimates are 0.018 m/d and 0.3 m/d.
- d. Peedee Formation: Hydraulic property estimates for this hydrogeologic unit are from 9.1 m/d to 69.2 m/d. The average storage coefficient for this aquifer is 4 x 10<sup>-4</sup>. According to Logan

and Euler (1988), the average transmissivity on site is  $1.1 \times 10^3$  m<sup>2</sup>/d.

- e. Williamsburg Formation: Hydraulic property measurements for this aquitard are available only from Area M. Horizontal hydraulic conductivities are in the range of 4.8 x 10<sup>-4</sup> m/d and 9.4 x 10<sup>-6</sup> m/d. Vertical hydraulic conductivities are assumed to be 2 orders of magnitude less. Over the majority of the site, the leakage coefficient (hydraulic conductivity/thickness) ranges from 10<sup>-4</sup>/day to 10<sup>-6</sup>/day.
- f. Congaree Formation: The transmissivity of this formation ranges from 1.5 m<sup>2</sup>/d to 9.3 x  $10^2$  m<sup>2</sup>/d, which indicates significant spatial variability within this aquifer. The storage coefficient is estimated as  $2 \times 10^{-4}$ .
- g. Tertiary Sand Aquifer: In general, this aquifer can be subdivided into the lower part (McBean Formation) and the upper part (Barnwell Formation) depending on the desired scale of the modeled domain. Root (1983) estimated that a hydraulic conductivity of about 1.8 m/d was necessary for proper calibration in the general separation area. The storage coefficient has a value of 1.2 x 10<sup>-4</sup> to 9.3 x 10-3 in the upper part and about 4.0 x 10<sup>-4</sup> for the lower part around Area H. Effective porosity is assumed to vary from 0.20 to 0.25.

Table 1 summarizes the hydraulic properties of the subsurface at the site. The horizontal hydraulic conductivity changes from 0.00095 m/hr on the lower aquitard to 1.04 m/hr on the lower aquifer. The ratio of horizontal hydraulic conductivity to the vertical conductivity was assumed to be 10 for the aquifer and 100 for the aquitard.

Table 1
Hydrologic Properties of Aquifers and Aquitards at SRS from the
Bottom (Layer 6) to Top (Layer 1)

	Formation	Hydraulic Conductivity, m/hr			
Layer		Horizontal	Vertical	Storage Coefficient	Porosity
ı	Middendorf	1.04	0.104	0.00045	0.30
2	Black Creek	0.028	0.00028	0.0004	N/A
3	PeeDee & BC	0.508	0.0508	0.00042	0.30
4	Williamsburg & Ellenton	0.00095	0.0000095	0.00001	N/A
5	Congaree	0.89	0.089	0.0002	0.20
6	McBean	0.127	0.0127	0.11	0.11

### Sources and Sinks

The flow in the SRS subsurface is controlled in part by infiltration (recharge) and pumping (discharge). A portion of the precipitation falling on the SRS infiltrates to the subsurface. Hubbard and Emslie<sup>1</sup> defined a water budget in the SRS. The amount of infiltration entering the aquiferaquitard system was calculated by subtracting surface runoff (7.6 cm/yr), evapotranspiration (76.2 cm/yr), and deep percolation (2.54 cm/yr) from precipitation (122 cm/yr). This leaves 35.6 cm/yr of water to become groundwater recharge. Hubbard (1986) suggested that the value of evapotranspiration in heavily forested areas might be much higher. Since the purpose of this project was to demonstrate the GMS capabilities rather than provide detailed results, a 35.6 cm/year recharge was considered to be reasonable. Figure 5 shows the estimated water balance at the Savannah River Site and vicinity.

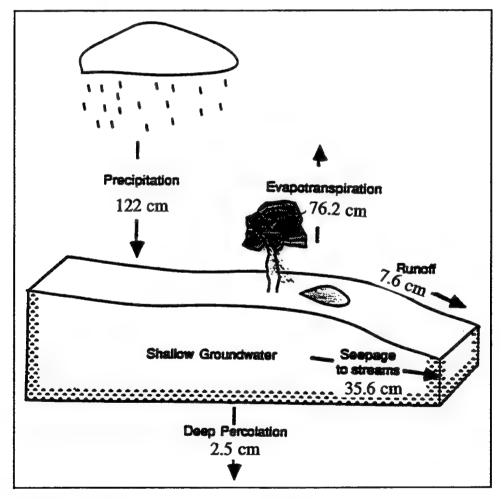


Figure 5. Hydrologic cycle and water budget at SRS (from Hubbard, Stephenson, Steele, and Gordon 1988)

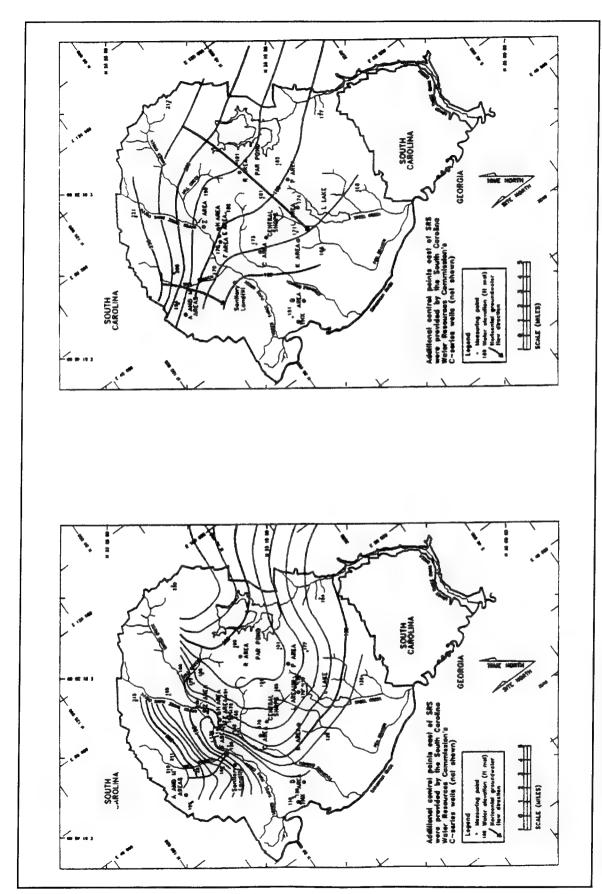
J. E. Hubbard and R. H. Emslie. (1984). Unpublished Manuscript, Savannah River Laboratory, Aiken, SC.

Groundwater pumpage is another important part of the hydrogeologic system at the SRS. Cristensen and Gordon (1983) identified 38 municipal and industrial production pumps within a 32-km (20-mile) radius of the center of SRS. It was reported that most of the 8.3 x 10<sup>5</sup> m³/d (21.9 mgd) total pumpage for these users was developed from the Middendorf, Black Creek, and PeeDee Formations. Only light pumpage occurs from Williamsburg and Ellenton Formations; it is small relative to those from the lower formation. From information such as Hubbard et al. (1988) and South Carolina state agencies, 14 significant production wells were identified, which were pumped at a rate from 34 to 513 m³/hr (Table 2 and Figure 4). The centers for greatest groundwater pumpage at SRS were A/M, F, and H areas.

Table 2 Pumping Rates Used for the SRS Regional Model				
	Pumping Rates			
Name	gpm	m³/hr		
Jackson	150	34		
Ellenton	400	91		
Area A/M	1,850	419		
Area F	1,760	398	•	
Area H	2,270	513		
Area C	200	45		
Area CS	200	45		
Area D	220	50		
Area K	620	140		
Area L	190	43		
Area P	240	54		
Williston	547	124		
Bamwell	1,693	383		
Sandoz Co.	1,321	299		

### **Hydrostratigraphic Framework**

Andersen et al. (1988) used potentiometric information of the site to determine the groundwater flow directions around the SRS. In the Middendorf aquifer, the groundwater flows north. In the vicinity of SRS, the Savannah River causes the groundwater to move in an acurate flow path (Figure 6) toward the river. A groundwater divide between the Savannah River and South Fork Edisto River is northeast of SRS. The groundwater flow direction in the Black Creek aguifer is similar to that of the Middendorf. In the Tertiary Sand Aquifer, the groundwater flow is dominated by the Savannah River. The resulting flow moves either west toward the Savannah River or east toward the South Fork Edisto River (passing outside the northeast corner 15 km away from the line Aiken to Williston). This flow pattern and other site characteristics described earlier were used as a foundation to develop the 3-D numerical model of SRS. Figure 6 represents the potentiometric surface and horizontal groundwater flow directions of the Congaree-Fourmile and Cretaceous zones at SRS during the first quarter of 1992 (Westinghouse Savannah River Company 1992).



Potentiometric surface and horizontal groundwater flow directions of the Congaree-Fourmile and Cretaceous Zones at SRS during the first quarter of 1992 (Westinghouse Savannah River Company 1992) Figure 6.

# 3 Numerical Model Development

GMS/FEMWATER was used for the model simulations at SRS. For detailed information on GMS and FEMWATER, the reader is referred to GMS (1994) and Lin, et al. (1997), respectively.

### FEMWATER

The computer code FEMWATER is a 3-D finite-element model for simulating flow and mass transport through saturated-unsaturated geologic formations. FEMWATER has several options that may be applied to the modeling of a wide range of real-world problems with flexibility and versatility. FEMWATER is based on a hybrid Lagrangian-Eulerian formulation that eliminates numerical oscillation due to high advective flow. Large time-steps can be used without causing numerical dispersion.

### **GMS** Interface

FEMWATER is incorporated into the Department of Defense Ground-water Modeling System (GMS). GMS is developed as a comprehensive graphical user environment for numerical modeling. The GMS has been developed with support from WES, the U.S. Army Environmental Center in Aberdeen, MD, in part by the EPA, AERL, and the U.S. Department of Energy. The GMS has numerical and graphical tools for site characterization, model conceptualization, mesh and grid generation, geostatistical calculations, and post-processing of output data. The numerical model described in this report uses the GMS interface and FEMWATER to demonstrate groundwater flow and transport modeling capability using the SRS as an example.

### Mesh generation

The surface area was divided into mesh elements using the two-dimensional (2-D) mesh module of GMS. The 2-D mesh is based on ground surface elevations, source/sink locations, hydraulic gradients, and historical flow lines. The surface elevations were taken from U.S. Geological Survey topographic sheets, and the surface mesh was generated using the WES Watershed Modeling System (WMS 1994). The boundaries of the model were extended beyond the SRS boundaries to eliminate errors due to the boundary condition specification.

Vertically, the model domain is divided into six layers of nonuniform thickness. Thicknesses were obtained from aquifer information and elevation maps of each of the hydrostatic units (Siple 1967 and Logan and Euler 1988). The front view of vertical elevation in the study area is shown in Figure 7. Vertical geologic profiles of the study area were defined from 11 sets of borehole data. The structure of borehole data and the 2-D mesh are shown in Figure 8. The domain is divided into four aquifers and two aquitards. The 3-D mesh (Figure 9) has 3864 elements and 2422 nodes.

### **Boundary conditions**

The boundary conditions for the SRS model basically correspond to permanent hydrologic boundaries. In this application, the permanent hydrologic boundaries include the Savannah River and the impermeable bedrock. It was assumed that the hydrologic system would not change significantly over the model simulation period near these boundaries. The boundary conditions for this application were the constant and spatial-varying total head along the model domain boundaries. Variable head boundary conditions were specified at 346 nodes based on interpolations and extrapolations of Andersen et al. (1988).

A specified flux condition with uniform distribution was applied to all active portions of the upper aquifer to represent recharge due to precipitation. Pumpage data for the major pumping locations were incorporated into the numerical model as specified flux boundary conditions. Locations of 14 individual pumping wells were initially superimposed onto the finite-element nodal points. In cases where the open interval of a well included several layers, the flux was assigned based on the length of the open interval for each affected layer. A total of 19 specified flux well nodes were used. The total pumpage in the model was 5.96 x 10<sup>2</sup> m<sup>3</sup>/l (2,638 gpm). Of this, 61 percent was from the Black Creek aquifer, and 28 percent was from the Middendorf aquifer.

Hydraulic conductivity was assumed to be homogeneous within each model layer. Although it is possible to estimate variation or zonation within the model, this demonstration of GMS did not attempt to address spatial variability. The subsurface material characteristics were included

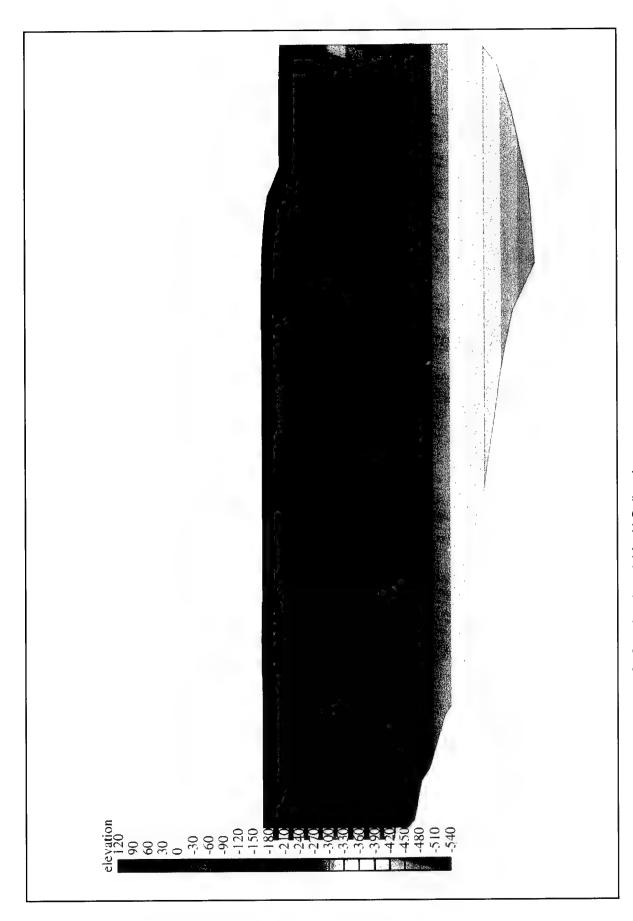


Figure 7. Front view of elevation at SRS regional model for N-S direction

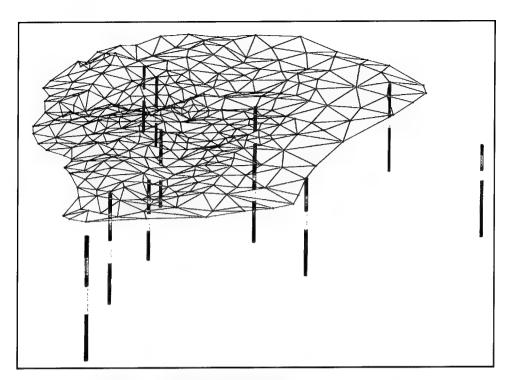


Figure 8. 2D mesh and borehole locations for SRS regional model

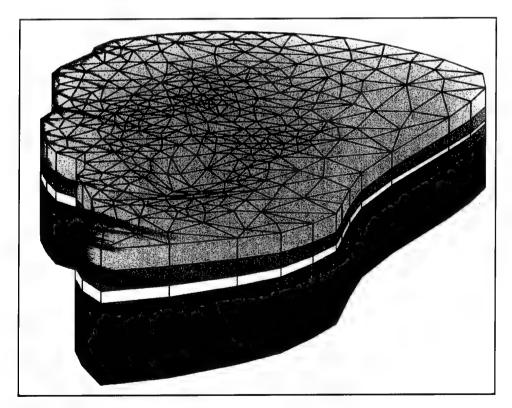


Figure 9. 3D computational mesh for SRS regional model

in the modeling by assigning the moisture content, relative conductivity, and water capacity for each model layer.

#### Initial conditions

In addition to the boundary conditions and other model input parameters, initial conditions needed to be assigned. For transient simulations, the initial conditions must be estimated using a field measurement or some estimation techniques. Since the field measurements of initial conditions were not available, a numerical procedure was developed to estimate initial conditions. Appropriate initial conditions make the convergence of the numerical model feasible and fast. A systematic iterative procedure was developed for generating initial conditions based on the above considerations. Initially, a constant head was used as initial condition and pressure heads were calculated for a period. The new calculated head then was used as initial conditions and simulations were repeated until a satisfactory initial condition was obtained.

#### Transient flow simulation

Using the estimated boundary and initial conditions, the model was run for a 1-year transient simulation with a variable time-step that varied from 0.5 to 5 hr. To demonstrate the effect of individual pumpage and infiltration on the flow system, three simulations of (a) a pumpage dominated system, (b) an infiltration dominated system, and (c) a pumpage and infiltration dominated system were performed. The simulated time-series of the pressure head and flow velocity were plotted to display the results. Two-dimensional (x-y) color contours of the pressure head and flow patterns were used to represent the dynamic changes of flow in each layer of the modeling domain. The basic finding of these three simulations are summarized as follows:

- a. One-year pumpage dominated simulation: At the end of the simulation, the flow follows a path towards lower elevations. Figure 10 shows this flow pattern for the top aquifer layer. Figure 11a illustrates the pressure head change for continuing pumping for the top aquifer. Decreases in the pressure head were observed in most areas of the model domain except at lower elevations where the pressure head increased compared to initial conditions. More significant influences of pumping were found around the higher pumping rate wells, such as A/M area, F area, Barnwell and Sandoz (Figure 4) for the third layer from the bottom (Figure 11b).
- b. One-year infiltration dominated simulation: A similar but more uniform flow pattern (Figure 12) was obtained as in the previous condition for the top aquifer layer at the end of simulation. The maximum increase of pressure head for both layer 1 (top layer) (Figure 13a) and layer 4 (from bottom) (Figure 13b) happened near

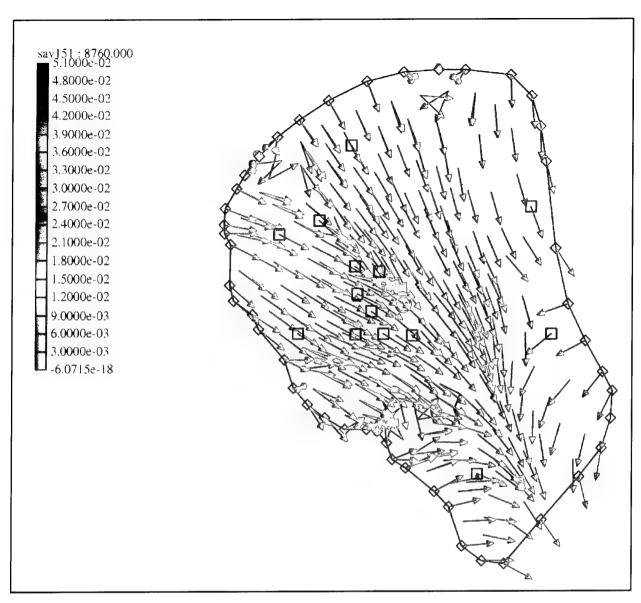


Figure 10. Simulated groundwater flow for top aquifer layer (the square boxes show the well locations at lower aquifer) at end of 1-year pumpage dominated simulation

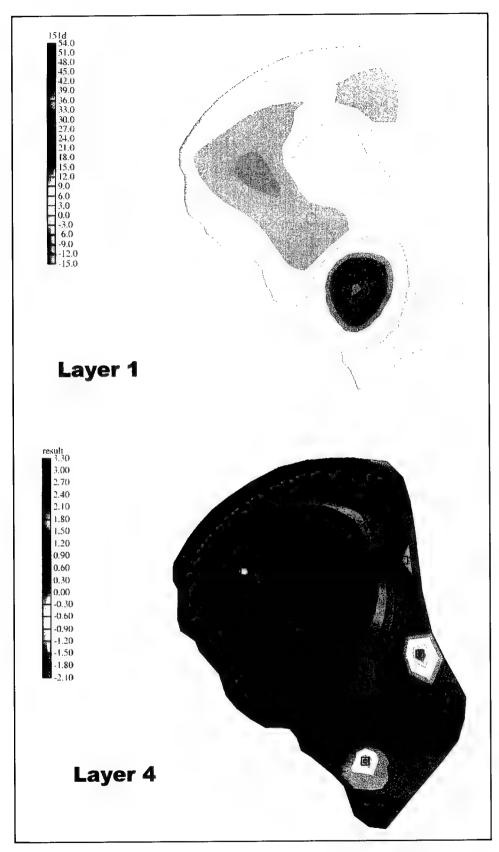


Figure 11. Difference of pressure head distribution between ending time and starting for 1-year pumpage dominated simulation

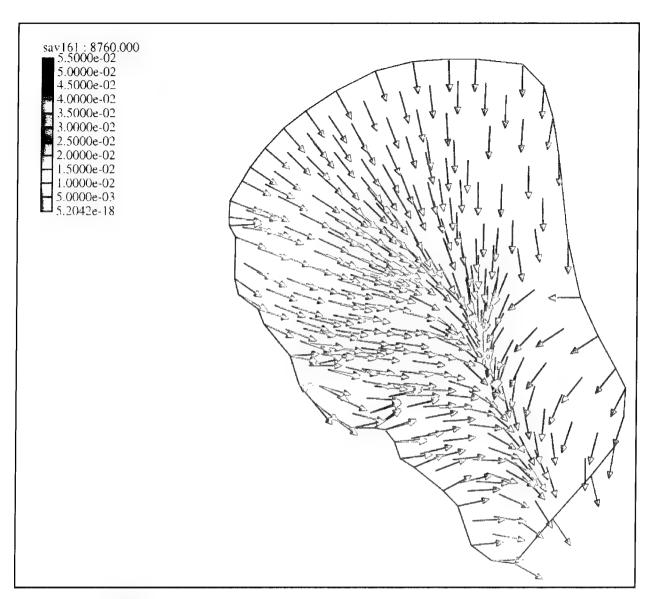


Figure 12. Simulated groundwater flow for top aquifer layer at end of 1-year infiltration dominated simulation

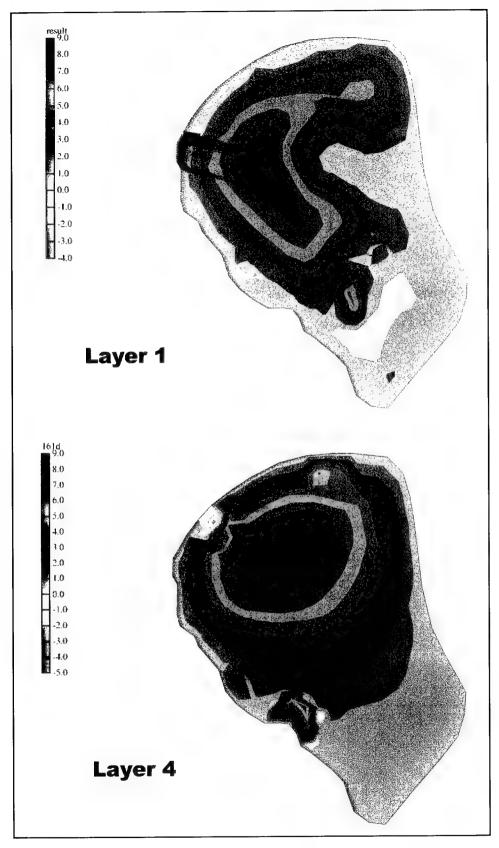


Figure 13. Difference of pressure head distribution between ending time and starting for 1-year infiltration dominated simulation

Tims Branch of the Upper Three Runs. The physical reason needs further study.

c. Two-year simulation with both pumpage and infiltration: Figure 14 (layer 1) shows a convergence of the lower elevation flow pattern for the combined pumping and infiltration factors. Although the model verification needs additional focus, the magnitude of simulated flow velocity has the same order as reported in the literature. While the top aquifer layer shows less variation in the pressure head, it was found that most of the modeled area increases the pressure head except those locations with more significant pumping effect (Figure 15a, layer 4). The pressure head in the bottom layer (layer 6) was dominated only by the hydraulic gradient (Figure 15b).

The mass balance of each of these flow simulations at hour 64 is summarized in Table 3. The results indicate that there was a significant nonlinearity in the flow system. It means that the mass balance for individual effects, such as infiltration and pumping, is not identical to the mass balance for combined factors. Figure 16 represents the differences of pressure head at the end of 1-year simulation in layer 1. From the similar pattern between Figures 16a and 16b, it can be shown that the pumping effect in this flow system was less significant than the infiltration effect.

Table 3 Mass Balance for Flow Simulation				
Factor	Infiltration, m/hr	Pumping, m <sup>3</sup> /hr	Infiltration and Pumping	
Flow through infiltration	-1.99e06	0.00e00	-1.54e06	
Flow through entire boundary	-5.73e06	-3.73e06	-3.76e06	
Artificial sources/sinks	0.00e00	1.68e05	1.68e05	
Increase in water content	4.06e06	5.07e05	1.08e06	

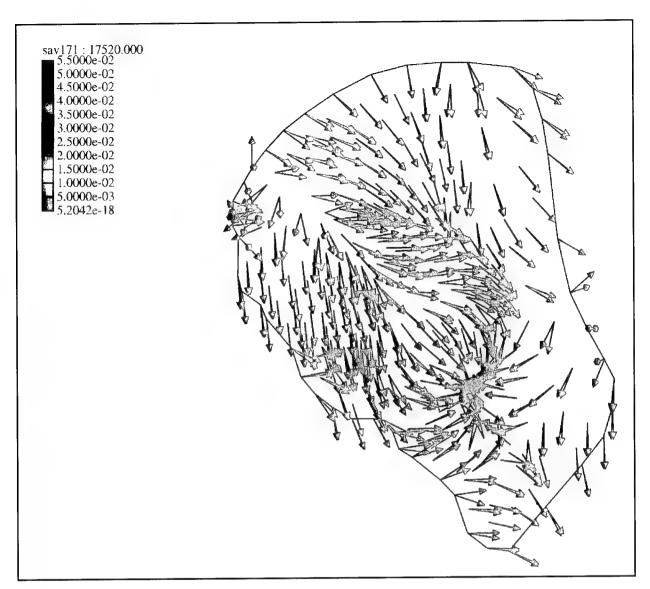


Figure 14. Simulated groundwater flow for top aquifer layer at end of 2-year combined factors

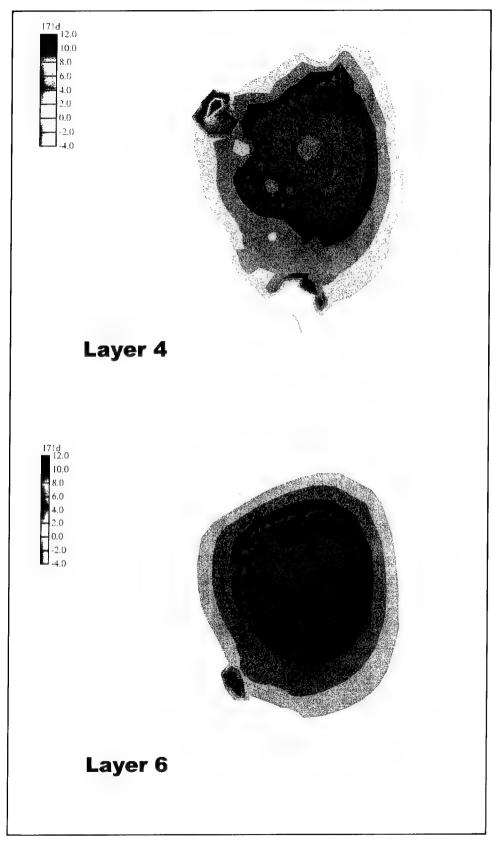


Figure 15. Difference of pressure head distribution between ending time and starting for 2-year combined factors

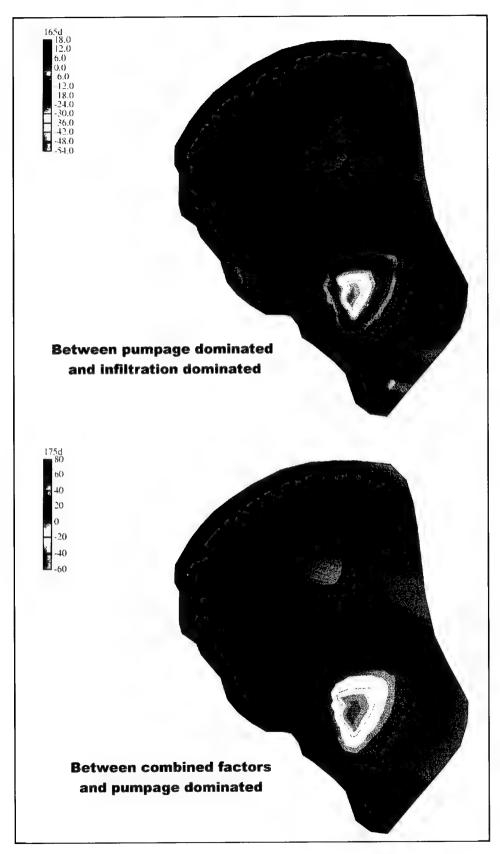


Figure 16. Difference of pressure head distribution for layer 1 at end of 1-year simulation (Continued)

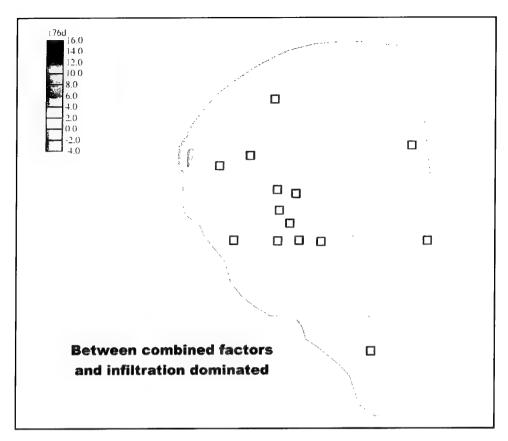


Figure 16. (Concluded)

### **Transport simulation**

One of the most important issues in this study was to predict the contaminant transport of tritium in the area. In the GMS, FEMWATER can be used with either coupled or decoupled flow and transport data. In this demonstration study, the decoupled option (separate flow and transport simulations) was used to examine the point source transport in the SRS. Tritium is the most abundant radionuclide present at the site. It was chosen to demonstrate the transport phenomena because it is present as atoms in water molecules and moves with the groundwater at the site as it decays. Tritium has a half-life of 12.3 years.

Using a distribution of tritium provided in Westinghouse Savannah River Company (1992), longitudinal (20-m) and lateral (2-m) dispersion coefficients were estimated. It was assumed that there was no molecular diffusion and that there were continuous sources in the five most active areas, primarily in the separation and waste management areas. The concentration at these locations was set to  $0.025\mu\text{Ci/ml}$  (Figure 17). The radioactive decay constant was computed as  $9.3 \times 10^{-6}$  from using the half-life period for tritium. A cross-sectional distribution of tritium is represented in Figure 18.

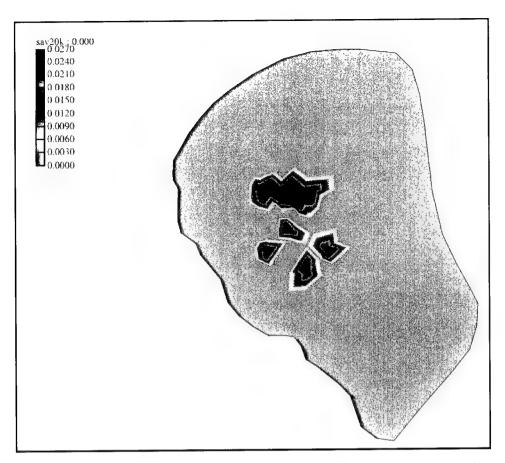


Figure 17. Sources of tritium concentrations for SRS regional model (top view)

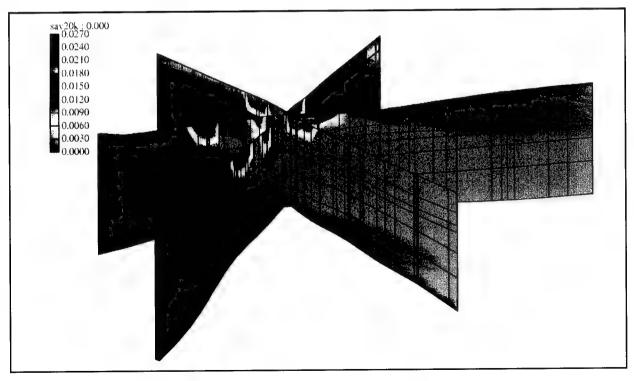


Figure 18. Cross-sectional view of tritium concentration sources for SRS regional model

A 2-year transport simulation was conducted using the initial and boundary conditions and flow velocity from the flow simulation. The distribution of tritium during these 2 years occurred only in the top layers. A display of the difference at the end of the simulation is presented in Figure 19a (layer 1) and Figure 19b (layer 2). The maximum concentration after 2 years was about 0.0008  $\mu Ci/ml$  at layer 1 and was 0.00025  $\mu Ci/ml$  at layer 2.

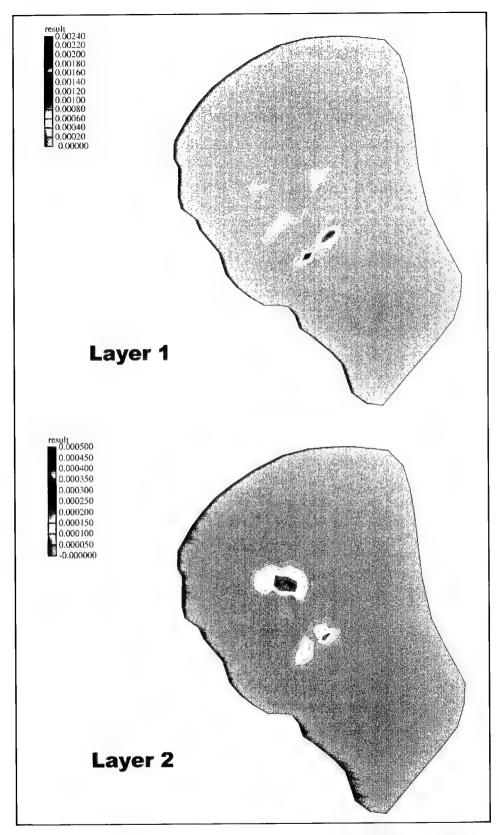


Figure 19. Difference of tritium concentration distribution between ending time and starting time for 2-year transport simulation. Results are given in uCi/ml

# 4 Conclusions

A FEMWATER model of the Savannah River Site project was successfully used to demonstrate the GMS/FEMWATER capability to model transient flow and transport from a point source of pollution. The highly irregular geometry of the site resulted in a slow numerical convergence of the flow simulation. The initial conditions of the flow and mass of tritium were crucial to completing the demonstration. The decoupled flow and transport capability of FEMWATER resulted in saving computational time in this study.

From this regional scale modeling study, it was determined that future refinements of the model mesh would be particularly important for addressing specific management issues. A new mesh should consider hydraulic and concentration gradients while providing reasonable stratigraphic representation and computational efficiency.

This modeling effort considered constant and spatially varying head boundary conditions over the model domain. Further studies should cover boundary uncertainty, incorporate time-varying fluxes, and include the stream-aquifer interaction options now available in the GMS/FEMWATER. These are necessary to address some unique groundwater flow features, such as flow reversal in the upper aquifer.

Parameter estimation techniques, including stochastic simulation, need to be considered in the numerical simulation. These numerical tools could be used for developing more comprehensive flow and transport systems, and for performing better model verification processes.

### References

- Andersen, Peter F., Sims, Paul N., Davis, Diane H., and Hughes, Shereen C. (1988). "A numerical model of the hydrogeological system underlying the Savannah River Plant," Prepared by GeoTrans, Inc., Herndon, VA, for Westinghouse Savannah River Company, Environmental Sciences Division, Savannah River Laboratory, Aiken, SC.
- Aucott, W. R. (1988). "The predevelopment and groundwater flow system and hydrologic characteristics of the Coastal Plain Aquifers of South Carolina," Water Resources Investigations Report 86-4347, U.S. Geological Survey, Columbia, SC.
- Aucott, W. R., Davis, M. E., and Speiran, G. K. (1987). "Geohydrologic framework of the Coastal Plan Aquifers of South Carolina," Water Resources Investigations Report 85-4271, U.S. Geological Survey, Columbia, SC.
- Christensen, E. J., and Gordon, D. E. (1983). "Technical summary of Groundwater Quality Protection Program at Savannah River Plant; Vol I: Site geohydrology and solid and hazardous wastes," DPST-83-829, E. I. du Pont de Nemours and Company, Savannah River Laboratory, Aiken, SC.
- Duffield, G. M., Buss, D. R., and Stephenson, D. E. (1990) "Velocity prediction errors related to flow model calibration uncertainty," ModelCAR 90: Calibration and Reliability in Groundwater Modeling, IAHS Publication No. 195, International Association of Hydrological Science, The Hague, The Netherlands.
- "Groundwater Modeling System (GMS) Reference Manual," (1994). GMS 1.2, Brigham Young University, Engineering Computer Graphics Laboratory, Provo, UT.
- Hubbard, J. E. (1986). "An update on the SRP Burial Ground Area water balance and hydrology," DPST-85-958, E. I. Du Pont de Nemours, Savannah River Laboratory, Aiken, SC.

- Hubbard, J. E., Stephenson, D. E., Steele, J. L., and Gordon, D. E.
  (1988). "Water resource management planning guide for Savannah
  River Plant," DPST-88-835, E. I. Du Pont de Nemours, Savannah River
  Laboratory, Aiken, SC.
- Lin, H. C. J., Richards, D. R., Yeh, G. T., Cheng, J. R., Cheng, H. P., and Jones, N. (1997). "FEMWATER - A three-dimensional finite-element computer model for simulating density-dependent flow and transport in variably saturated media," Technical Report CHL-97-12, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.
- Logan, Robert W., and Euler, Gwen M. (1988). "Geology and groundwater resources, Allendale, Bamberg and Barnwell Counties and part of the Aiken County South Carolina," Water Resources Commission Report No. 155, State of South Carolina, Columbia, SC.
- Root, R.W., Jr. (1983). "Numerical modeling of groundwater flow at the Savannah River Plant," S DOE Report DP-1638, Aiken, SC.
- Siple, G. E. (1967). "Geology and groundwater of the Savannah River plant and vicinity, South Carolina," Water Supply Paper 1841, U.S. Geological Survey, Columbia, SC.
- "Watershed Modeling System (WMS) (1994 Version), WMS Reference Manual," (1994). Brigham Young University, Engineering Computer Graphics Laboratory, Provo, UT.
- Westinghouse Savannah River Company. (1992). "Savannah River Site environmental report for 1992," Environmental Monitoring Section, Westinghouse Savannah River Company, Department of Energy, Savannah River Site, Aiken, SC.
- Yeh, G. T. (1994). "User's manual: A three-dimensional finite element model of water flow through saturated-unsaturated media," Pennsylvania State University, PA.

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#### 13. ABSTRACT (Maximum 200 words)

A numerical simulation of a site at the Savannah River Site is presented to demonstrate the GMS/FEMWATER capabilities. Tritium was selected as the chemical of concern for the transport simulation. Effects of the hydrogeologic parameters such as infiltration and pumping on the flow and tritium transport were investigated. The highly irregular geometry of the site resulted in a slow numerical convergence of the flow simulations. The initial conditions of the flow and mass of the tritium were crucial to this demonstration. The future modeling of the site should include a detailed mesh system, sufficient hydrogeologic and chemical data, and incorporation of a parameter estimation technique.

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